#### metal-organic compounds



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# catena-Poly[[silver(I)- $\mu$ -N-(pyridin-3-yl-methyl)pyridine-2-amine- $\kappa^2 N$ :N'] trifluoromethanesulfonate]

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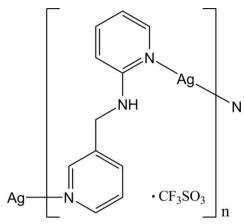
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Key indicators: single-crystal X-ray study; T = 173 K; mean  $\sigma(C-C) = 0.017$  Å; R factor = 0.088; wR factor = 0.238; data-to-parameter ratio = 14.0.

In the asymmetric unit of the title polymeric complex,  $\{[Ag(C_{11}H_{11}N_3)](CF_3SO_3)\}_n$ , there are two  $Ag^I$  atoms, two N-(pyridin-3-ylmethyl)pyridine-2-amine ligands (A and B) and two CF<sub>3</sub>SO<sub>3</sub><sup>-</sup> anions. One Ag<sup>I</sup> atom is coordinated by two pyridine N atoms from two symmetry-related A ligands in a geometry slightly distorted from linear [N-Ag-N = 173.2 (3)°], forming a left-handed helical chain, while the other Ag<sup>I</sup> atom is coordinated by two pyridine N atoms from two symmetry-related B ligands in a bent arrangement [N- $Ag-N = 157.1 (3)^{\circ}$ , forming a right-handed helical chain. Both helical chains have the same pitch length [10.4007 (7) Å], propagate along the b-axis direction and are alternately arranged via Ag···Ag [3.0897 (12) Å] and  $\pi$ – $\pi$  stacking interactions [centroid-centroid distances = 3.564 (7) and 3.518 (6) Å], resulting in the formation of a two-dimensional supramolecular network extending parallel to the ab plane. Intermolecular  $N-H\cdots O$ ,  $C-H\cdots O$  and  $C-H\cdots F$ hydrogen-bonding interactions occur between the helical chains and the anions.

#### **Related literature**

For related structures and applications of Ag<sup>I</sup> coordination polymers with dipyridyl ligands, see: Leong & Vittal (2011); Moulton & Zaworotko (2001). For the crystal structure of the related perchlorate salt, see: Zhang *et al.* (2013). For the synthesis of the ligand, see: Foxon *et al.* (2002); Lee *et al.* (2008).



#### **Experimental**

#### Crystal data

$[Ag(C_{11}H_{11}N_3)](CF_3O_3S)$	$V = 2951.4 (4) \text{ Å}^3$
$M_r = 442.17$	Z = 8
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 14.0965 (10)  Å	$\mu = 1.56 \text{ mm}^{-1}$
b = 10.4007 (7)  Å	T = 173  K
c = 20.6593 (15)  Å	$0.30 \times 0.25 \times 0.25 \text{ mm}$
$\beta = 102.994 (1)^{\circ}$	

#### Data collection

Bruker SMART CCD area-detector diffractometer 5797 ind Absorption correction: multi-scan (SADABS; Bruker, 2000)  $R_{int} = 0.652, T_{max} = 0.697$  16169 m 5797 ind 4479 refl 4479 refl 479 r

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.088$   $wR(F^2) = 0.238$  S = 1.095797 reflections 415 parameters 16169 measured reflections 5797 independent reflections 4479 reflections with  $I > 2\sigma(I)$   $R_{\rm int} = 0.047$ 

6 restraints

H-atom parameters constrained  $\Delta \rho_{\text{max}} = 2.70 \text{ e Å}^{-3}$   $\Delta \rho_{\text{min}} = -1.89 \text{ e Å}^{-3}$ 

**Table 1** Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	D-H	$H \cdot \cdot \cdot A$	$D \cdot \cdot \cdot A$	$D-H\cdots A$
N3—H3···O4	0.88	2.20	3.021 (12)	156
$N6-H6\cdots O2^{i}$	0.88	2.42	3.159 (12)	142
C1-H1···O1	0.95	2.56	3.389 (16)	146
$C6-H6A\cdots F6^{ii}$	0.99	2.55	3.282 (15)	131
C9−H9···O3 <sup>iii</sup>	0.95	2.44	3.329 (14)	156
$C10-H10\cdots O1^{iv}$	0.95	2.57	3.373 (14)	142
$C12-H12\cdots O4^{v}$	0.95	2.51	3.331 (15)	145
$C17-H17A\cdots O3^{i}$	0.99	2.42	3.186 (14)	134
$C21-H21\cdots F6^{vi}$	0.95	2.54	3.325 (14)	140

Symmetry codes: (i) -x,  $y-\frac{1}{2}$ ,  $-z+\frac{1}{2}$ ; (ii) x,  $-y+\frac{3}{2}$ ,  $z+\frac{1}{2}$ ; (iii) x+1,  $-y+\frac{3}{2}$ ,  $z+\frac{1}{2}$ ; (iv) -x+1,  $y-\frac{1}{2}$ ,  $-z+\frac{1}{2}$ ; (v) x-1, y, z; (vi) -x+1,  $y+\frac{1}{2}$ ,  $-z+\frac{1}{2}$ .

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

### metal-organic compounds

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SJ5332).

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Acta Cryst. (2013). E69, m414-m415 [doi:10.1107/S1600536813016309]

## *catena*-Poly[[silver(I)- $\mu$ -N-(pyridin-3-ylmethyl)pyridine-2-amine- $\kappa^2 N$ :N'] tri-fluoromethanesulfonate]

#### **Suk-Hee Moon and Ki-Min Park**

#### Comment

Silver coordination polymers based on dipyridyl type ligands have attracted particular interest because of the intriguing architectures caused by a variety of coordination geometries for the Ag(I) cation as well as their potential applications as functional materials (Leong & Vittal, 2011; Moulton & Zaworotko, 2001). However, despite the rapid growth in the Ag(I) coordination chemistry based on symmetrical dipyridyl ligands, investigations using unsymmetrical dipyridyl ligands with nitrogen donor atoms in different positions on the two terminal pyridines still remains lacking. Herein, we report the crystal structure of the title compound prepared by the reaction of silver trifluoromethanesulfonate with the unsymmetrical dipyridyl ligand. The structure of title compound is isostructural with the perchlorate salt (Zhang *et al.*, 2013).

The asymmetric unit of the title compound contains two Ag<sup>I</sup> atoms (Ag1 and Ag2), two *N*-(pyridin-3-ylmethyl)-pyridine-2-amine (Foxon *et al.*, 2002; Lee *et al.*, 2008) ligands (A and B) and two CF<sub>3</sub>SO<sub>3</sub><sup>-</sup> anions. The Ag1 atom is coordinated by two pyridine N atoms from two symmetry-related ligand A in a geometry slightly distorted from linear [N-Ag1-N = 173.2 (3)°] to form left-handed helical chain, while the Ag2 atom is coordinated by two pyridine N atoms from two symmetry-related ligand B in a bent arrangement [N-Ag2-N = 157.1 (3)°] to form right-handed helical chain (Fig. 1). Two pyridine rings coordinated to the Ag1 and Ag2 centers are tilted by 14.2 (7)° and 34.1 (5)°, respectively, with respect to each other. Both helical chains with the same pitch length of 10.4007 (7) Å propagate along the *b* axis and are alternately arranged *via* the Ag···Ag interactions [3.0897 (12) Å], resulting in the formation of a two-dimensional supramolecular network extending parallel to the *ab* plane. Furthermore,  $\pi$ - $\pi$  stacking interactions [centroid-centroid distances = 3.564 (7) and 3.518 (6) Å] between pyridine rings of both helical chains, as shown in Fig. 2, contribute to stabilize the two-dimensional network.

The non-coordinating  $CF_3SO_3$  anions participate in N–H···O hydrogen bonding (Table 1, Fig. 2) and Ag···O interactions (Ag1···O4 2.815 (8), Ag1···O5 2.852 (10), Ag1···O1 2.867 (8), Ag2···O2 2.722 (8) Å) (Fig. 1,2). In addition, C–H···O and C–H···F hydrogen bonds (Table 1) between the helical chains and anions are also detected in the crystal.

#### **Experimental**

The ligand (*N*-(pyridin-3-ylmethyl)pyridine-2-amine) was prepared according to a procedure described by Foxon *et al.* (2002). Crystals of the title compound suitable for X-ray analysis were obtained by vapor diffusion of diethyl ether into a DMSO solution of the white precipitate afforded by the reaction of the ligand with silver(I) trifluoromethanesulfonate in a 1:1 molar ratio in methanol.

#### Refinement

All H atoms were positioned geometrically and refined using a riding model, with d(C-H) = 0.95 Å for  $Csp^2$ -H, 0.88 Å for amine N-H and 0.99 Å for methylene C-H. For all H atoms  $U_{iso}(H) = 1.2U_{eq}(C,N)$ .

#### **Computing details**

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT-Plus* (Bruker, 2000); data reduction: *SAINT-Plus* (Bruker, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

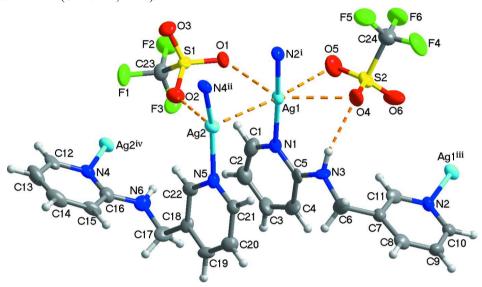


Figure 1

A view of the molecular structure of the title compound, with atom numbering. Displacement ellipsoids are drawn at the 50% probability level and dashed lines present Ag···O and N–H···O contacts. [Symmetry codes: (i) 1 - x, 1/2 + y, 1/2 - z; (ii) -x, 1/2 + y, 1/2 - z; (iii) 1 - x, -1/2 + y, 1/2 - z; (iv) -x, -1/2 + y, 1/2 - z].

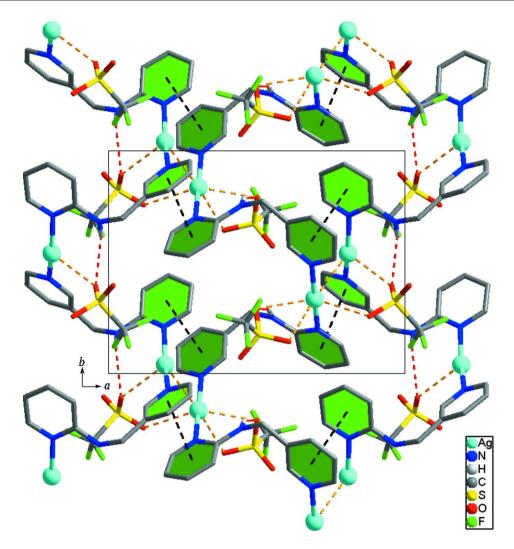


Figure 2 The two-dimensional supramolecular structure formed through Ag···Ag and Ag···O interactions (yellow dashed lines) and  $\pi$ - $\pi$  stacking interactions (black dashed lines). Red dashed lines present N-H···O hydrogen bonds.

#### *catena*-Poly[[silver(I)- $\mu$ -N-(pyridin-3-ylmethyl)pyridine-2-amine- $\kappa$ <sup>2</sup>N:N'] trifluoromethanesulfonate]

#### Crystal data

F(000) = 1744 $[Ag(C_{11}H_{11}N_3)](CF_3O_3S)$  $M_r = 442.17$  $D_{\rm x} = 1.990 {\rm \ Mg \ m^{-3}}$ Monoclinic,  $P2_1/c$ Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å Hall symbol: -P 2ybc Cell parameters from 5912 reflections a = 14.0965 (10) Å $\theta$  = 2.2–28.1°  $\mu = 1.56 \text{ mm}^{-1}$ b = 10.4007 (7) ÅT = 173 Kc = 20.6593 (15) Å $\beta = 102.994 (1)^{\circ}$ Block, colourless  $V = 2951.4 (4) \text{ Å}^3$  $0.30\times0.25\times0.25~mm$ Z = 8

*Acta Cryst.* (2013). **E69**, m414–m415 **Sup-3** 

#### Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan

Absorption correction: multi-scan (SADABS; Bruker, 2000)  $T_{\text{min}} = 0.652$ ,  $T_{\text{max}} = 0.697$ 

#### Refinement

Refinement on  $F^2$ Least-squares matrix: full  $R[F^2 > 2\sigma(F^2)] = 0.088$   $wR(F^2) = 0.238$  S = 1.095797 reflections 415 parameters 6 restraints Primary atom site location: structure-invariant direct methods 16169 measured reflections 5797 independent reflections 4479 reflections with  $I > 2\sigma(I)$   $R_{\text{int}} = 0.047$   $\theta_{\text{max}} = 26.0^{\circ}, \, \theta_{\text{min}} = 1.5^{\circ}$   $h = -17 \rightarrow 14$   $k = -12 \rightarrow 12$   $l = -15 \rightarrow 25$ 

Secondary atom site location: difference Fourier map Hydrogen site location: inferred from neighbouring sites H-atom parameters constrained  $w = 1/[\sigma^2(F_o^2) + (0.1255P)^2 + 38.027P]$  where  $P = (F_o^2 + 2F_c^2)/3$   $(\Delta/\sigma)_{\text{max}} = 0.001$   $\Delta\rho_{\text{max}} = 2.70 \text{ e Å}^{-3}$   $\Delta\rho_{\text{min}} = -1.89 \text{ e Å}^{-3}$ 

#### Special details

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted R-factor wR and goodness of fit S are based on  $F^2$ , conventional R-factors R are based on F, with F set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on  $F^2$  are statistically about twice as large as those based on F, and F-factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters  $(\mathring{A}^2)$ 

	X	у	Z	$U_{ m iso}$ */ $U_{ m eq}$	
Agl	0.30400 (6)	0.83549 (8)	0.19418 (4)	0.0296 (3)	
Ag2	0.19133 (6)	1.03934 (8)	0.25579 (4)	0.0301 (3)	
N1	0.2935 (6)	0.6974 (8)	0.2706 (4)	0.0255 (19)	
N2	0.6866 (6)	0.4901 (9)	0.3732 (5)	0.029 (2)	
N3	0.4482 (7)	0.7530 (10)	0.3296 (4)	0.037 (2)	
Н3	0.4585	0.7873	0.2929	0.045*	
N4	-0.1876 (6)	0.7099(8)	0.3036 (4)	0.0268 (19)	
N5	0.2011 (6)	0.9267 (9)	0.3454 (5)	0.029 (2)	
N6	-0.0305 (7)	0.6806 (9)	0.3627 (5)	0.031 (2)	
Н6	-0.0245	0.6207	0.3338	0.037*	
C1	0.2165 (9)	0.6290 (13)	0.2671 (7)	0.045 (3)	
H1	0.1679	0.6390	0.2273	0.053*	
C2	0.1944 (9)	0.5454 (12)	0.3110(7)	0.041 (3)	
H2	0.1341	0.5008	0.3038	0.049*	
C3	0.2670 (9)	0.5300 (13)	0.3677 (7)	0.045 (3)	
H3A	0.2579	0.4718	0.4012	0.055*	
C4	0.3531 (10)	0.5987 (12)	0.3761 (6)	0.041 (3)	

H4	0.4029	0.5883	0.4152	0.050*
C5	0.3656 (8)	0.6842 (10)	0.3259 (5)	0.028(2)
C6	0.5209 (9)	0.7732 (12)	0.3911 (6)	0.041(3)
H6A	0.4884	0.7677	0.4288	0.050*
H6B	0.5474	0.8613	0.3908	0.050*
C7	0.6058 (8)	0.6777 (10)	0.4031 (5)	0.027(2)
C8	0.6852 (8)	0.6987 (10)	0.4541 (6)	0.030(2)
Н8	0.6856	0.7712	0.4821	0.036*
C9	0.7637 (8)	0.6182 (11)	0.4657 (5)	0.031(2)
Н9	0.8177	0.6327	0.5017	0.038*
C10	0.7620(8)	0.5156 (11)	0.4235 (5)	0.028(2)
H10	0.8170	0.4603	0.4305	0.034*
C11	0.6099 (8)	0.5723 (11)	0.3626 (5)	0.030(2)
H11	0.5568	0.5571	0.3260	0.036*
C12	-0.2713 (9)	0.7802 (10)	0.2889 (6)	0.031(2)
H12	-0.3248	0.7489	0.2562	0.037*
C13	-0.2807 (10)	0.8951 (12)	0.3200 (7)	0.044(3)
H13	-0.3400	0.9421	0.3097	0.053*
C14	-0.2031 (10)	0.9394 (11)	0.3658 (6)	0.042(3)
H14	-0.2082	1.0195	0.3868	0.051*
C15	-0.1179 (9)	0.8727 (10)	0.3827 (5)	0.030(3)
H15	-0.0641	0.9046	0.4151	0.036*
C16	-0.1127 (8)	0.7554 (10)	0.3505 (6)	0.030(2)
C17	0.0462 (9)	0.6965 (11)	0.4212 (6)	0.035 (3)
H17A	0.0770	0.6118	0.4336	0.041*
H17B	0.0171	0.7252	0.4581	0.041*
C18	0.1260 (7)	0.7931 (9)	0.4138 (5)	0.024 (2)
C19	0.1999 (8)	0.8217 (10)	0.4677 (5)	0.028 (2)
H19	0.1992	0.7871	0.5102	0.034*
C20	0.2750 (9)	0.9011 (11)	0.4598 (6)	0.034 (3)
H20	0.3263	0.9219	0.4966	0.040*
C21	0.2744 (8)	0.9506 (10)	0.3966 (5)	0.029 (2)
H21	0.3273	1.0021	0.3904	0.034*
C22	0.1266 (8)	0.8491 (10)	0.3534 (5)	0.027 (2)
H22	0.0740	0.8333	0.3165	0.032*
S1	0.03282 (18)	0.8243 (2)	0.12350 (13)	0.0236 (5)
O1	0.1186 (5)	0.7565 (7)	0.1159 (4)	0.0321 (17)
O2	0.0432 (6)	0.8922 (7)	0.1865 (4)	0.0351 (18)
O3	-0.0157 (6)	0.8948 (7)	0.0660 (4)	0.0353 (18)
C23	-0.0529 (8)	0.6965 (11)	0.1288 (6)	0.033 (3)
F1	-0.1388 (5)	0.7438 (7)	0.1347 (4)	0.0483 (19)
F2	-0.0687 (6)	0.6231 (7)	0.0747 (4)	0.0506 (19)
F3	-0.0193 (5)	0.6218 (7)	0.1815 (4)	0.0451 (18)
S2	0.4912 (2)	0.6737 (3)	0.15718 (15)	0.0355 (7)
O4	0.5019 (6)	0.7902 (9)	0.1973 (4)	0.0333 (7)
O5	0.3907 (6)	0.6430 (10)	0.1279 (5)	0.043 (2)
06	0.5539 (7)	0.5725 (8)	0.1279 (3)	0.033 (2)
C24	0.5353 (10)	0.7271 (13)	0.0856 (7)	0.046 (2)
F4	0.6289 (5)	0.7586 (8)	0.1038 (4)	0.046 (3)
17	0.0209 (3)	0.7300 (0)	0.1030 (4)	0.030 (2)

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F5	0.4872 (7)	0.8264 (8)	0.0557 (4)	0.067 (3)
F6	0.5285 (6)	0.6260 (8)	0.0427 (4)	0.055 (2)

Atomic displacement parameters  $(\mathring{A}^2)$ 

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Agl	0.0285 (4)	0.0302 (5)	0.0323 (5)	0.0106 (3)	0.0116 (3)	0.0109 (3)
Ag2	0.0345 (5)	0.0296 (5)	0.0286 (5)	0.0019(3)	0.0124(3)	0.0066(3)
N1	0.028 (5)	0.018 (4)	0.032 (5)	0.009(4)	0.010(4)	0.006(4)
N2	0.024 (5)	0.033 (5)	0.030 (5)	0.002 (4)	0.010(4)	-0.003(4)
N3	0.042(6)	0.049 (6)	0.020(5)	0.014 (5)	0.006(4)	0.017(4)
N4	0.033 (5)	0.024 (4)	0.027 (5)	-0.002(4)	0.014 (4)	-0.001(4)
N5	0.019(4)	0.031 (5)	0.036 (5)	-0.001(4)	0.006(4)	0.001(4)
N6	0.034 (5)	0.024 (5)	0.035 (5)	-0.011(4)	0.005 (4)	-0.001(4)
C1	0.031 (7)	0.047(8)	0.052(8)	0.006(6)	0.002(6)	0.005 (6)
C2	0.038 (7)	0.034 (7)	0.055 (8)	0.001 (5)	0.018 (6)	0.005 (6)
C3	0.037(7)	0.052(8)	0.054(8)	0.007(6)	0.024(6)	0.022(7)
C4	0.047(7)	0.039(7)	0.039 (7)	0.026 (6)	0.011 (6)	0.017 (6)
C5	0.027 (5)	0.027(6)	0.034(6)	0.014 (4)	0.015 (5)	0.001 (4)
C6	0.046 (7)	0.040 (7)	0.037 (7)	0.015 (6)	0.005 (6)	-0.004(5)
C7	0.026 (5)	0.029(6)	0.026 (5)	0.002 (4)	0.008 (4)	0.003 (4)
C8	0.033 (6)	0.025 (5)	0.035 (6)	-0.009(5)	0.015 (5)	0.001 (5)
C9	0.029 (6)	0.041 (6)	0.022 (5)	-0.004(5)	0.004 (4)	-0.001(5)
C10	0.025 (5)	0.037 (6)	0.024 (5)	0.002 (5)	0.008 (4)	0.003 (5)
C11	0.027 (6)	0.034 (6)	0.030(6)	-0.018(5)	0.008 (5)	0.001 (5)
C12	0.042 (6)	0.024 (5)	0.035 (6)	0.003 (5)	0.026 (5)	0.010 (5)
C13	0.054 (8)	0.028 (6)	0.061 (8)	-0.001 (6)	0.037 (7)	-0.004 (6)
C14	0.066 (9)	0.024 (6)	0.047 (7)	-0.017 (6)	0.034 (7)	-0.011 (5)
C15	0.048 (7)	0.017 (5)	0.029 (6)	-0.017 (5)	0.020 (5)	-0.010 (4)
C16	0.032 (6)	0.027 (6)	0.036 (6)	-0.004(5)	0.014 (5)	0.001 (5)
C17	0.039 (5)	0.029 (5)	0.036 (5)	-0.015 (4)	0.008 (4)	0.010(4)
C18	0.025 (5)	0.009 (4)	0.035 (6)	0.000 (4)	0.003 (4)	0.000(4)
C19	0.043 (6)	0.021 (5)	0.020 (5)	0.001 (5)	0.006 (5)	0.004 (4)
C20	0.039 (6)	0.026 (6)	0.034 (6)	-0.004(5)	0.006 (5)	-0.002(5)
C21	0.024 (5)	0.031 (6)	0.031 (6)	0.001 (4)	0.008 (5)	0.004 (5)
C22	0.033 (6)	0.021 (5)	0.027 (5)	-0.003(4)	0.008 (5)	-0.003 (4)
S1	0.0243 (12)	0.0202 (12)	0.0250 (13)	-0.0021 (10)	0.0031 (10)	0.0036 (10)
O1	0.024 (4)	0.036 (4)	0.039 (4)	0.004(3)	0.014(3)	0.006 (4)
O2	0.044 (5)	0.029 (4)	0.033 (4)	-0.009(4)	0.009 (4)	-0.006(3)
О3	0.042 (5)	0.027 (4)	0.035 (4)	0.004(3)	0.005 (4)	0.013 (3)
C23	0.029 (6)	0.026(6)	0.043 (7)	-0.004(5)	0.009 (5)	0.002 (5)
F1	0.022(3)	0.051 (4)	0.074 (5)	-0.002(3)	0.016 (3)	0.013 (4)
F2	0.065 (5)	0.036 (4)	0.049 (4)	-0.012 (4)	0.008 (4)	-0.020(3)
F3	0.039 (4)	0.034 (4)	0.061 (5)	-0.001 (3)	0.008(3)	0.026(3)
S2	0.0376 (16)	0.0334 (15)	0.0401 (16)	0.0023 (12)	0.0185 (13)	0.0078 (12
O4	0.039 (5)	0.052 (5)	0.039 (5)	0.014 (4)	0.013 (4)	-0.014 (4)
O5	0.036 (5)	0.060 (6)	0.068 (7)	-0.017 (4)	0.020 (5)	-0.007(5)
O6	0.078 (7)	0.029 (4)	0.034 (5)	0.014 (4)	0.017 (4)	0.005 (4)
C24	0.050 (8)	0.045 (8)	0.044 (7)	0.006 (6)	0.015 (6)	0.009 (6)
F4	0.046 (4)	0.057 (5)	0.077 (6)	-0.020 (4)	0.039 (4)	-0.005(4)

F5 F6	0.090 (7) 0.070 (5)	0.061 (5) 0.056 (5)	0.054 (5) 0.041 (4)	0.032 (5) 0.014 (4)	0.029 (5) 0.016 (4)	0.038 (4) -0.016 (4)
	0.070 (3)	0.030 (3)	0.041 (4)	0.014 (4)	0.010 (4)	0.010 (4)
Geome	etric parameters (2	Å, °)				
Ag1—	N2i	2.151	(9)	С9—Н9		0.9500
Ag1—		2.164	* *	C10—H10		0.9500
Ag1—	Ag2	3.0897	7(12)	C11—H11		0.9500
Ag2—	N4 <sup>ii</sup>	2.151	(9)	C12—C13		1.378 (17)
Ag2—]	N5	2.169	(9)	C12—H12		0.9500
N1—C	21	1.286	(16)	C13—C14		1.36 (2)
N1—C	25	1.355	(14)	C13—H13		0.9500
N2—C	210	1.336	(14)	C14—C15		1.362 (18)
N2—C	C11	1.357	(15)	C14—H14		0.9500
N2—A	kg1 <sup>iii</sup>	2.151	(9)	C15—C16		1.399 (15)
N3—C	25	1.354	(15)	C15—H15		0.9500
N3—C	C6	1.458		C17—C18		1.541 (14)
N3—H	I3	0.8800	)	C17—H17A		0.9900
N4—C	216	1.348	(14)	C17—H17B		0.9900
N4—C	212	1.363	(14)	C18—C19		1.376 (15)
N4—A	ag2iv	2.151	(9)	C18—C22		1.378 (15)
N5—C	221	1.325	(14)	C19—C20		1.382 (16)
N5—C	222	1.364	(14)	C19—H19		0.9500
N6—C	216	1.371	(15)	C20—C21		1.401 (16)
N6—C	217	1.437	(14)	C20—H20		0.9500
N6—H	16	0.8800	)	C21—H21		0.9500
C1—C	22	1.343	(19)	C22—H22		0.9500
C1—H	[1	0.9500	)	S1—O3		1.432 (8)
C2—C	23	1.380	(19)	S1—O1		1.439 (8)
C2—H	[2	0.9500	)	S1—O2		1.459 (8)
C3—C	24	1.385	(19)	S1—C23		1.817 (11)
С3—Н	[3A	0.9500	)	C23—F2		1.331 (14)
C4—C	25	1.406	(16)	C23—F3		1.335 (13)
C4—H	[4	0.9500	)	C23—F1		1.338 (13)
C6—C	27	1.532	(15)	S2—O6		1.408 (9)
C6—H	[6A	0.9900	)	S2—O5		1.445 (9)
C6—H	16B	0.9900	)	S2—O4		1.457 (9)
C7—C	28	1.370	(15)	S2—C24		1.815 (13)
C7—C	211	1.388	(16)	C24—F5		1.312 (15)
C8—C	9	1.365	(16)	C24—F4		1.329 (15)
C8—H	[8	0.9500	)	C24—F6		1.365 (16)
C9—C	210	1.374	(16)			
	Ag1—N1	173.2	(3)	N4—C12—C13		122.1 (12)
N2 <sup>i</sup> —A	Ag1—Ag2	82.3 (2	2)	N4—C12—H12		118.9
N1—A	Ag1—Ag2	91.7 (2	2)	C13—C12—H12		118.9
N4 <sup>ii</sup> —	Ag2—N5	157.1	(3)	C14—C13—C12		118.1 (13)
N4 <sup>ii</sup> —	Ag2—Ag1	106.3	(2)	C14—C13—H13		120.9
N5—A	ag2—Ag1	92.4 (2	2)	C12—C13—H13		120.9
C1—N	11—C5	117.0	(10)	C13—C14—C15		122.2 (11)

C1—N1—Ag1	121.4 (8)	C13—C14—H14	118.9
C5—N1—Ag1	121.4 (7)	C15—C14—H14	118.9
C10—N2—C11	117.8 (9)	C14—C15—C16	117.3 (11)
C10—N2—Ag1 <sup>iii</sup>	119.9 (7)	C14—C15—H15	121.3
C11—N2—Ag1 <sup>iii</sup>	122.0 (7)	C16—C15—H15	121.3
C5—N3—C6	123.5 (10)	N4—C16—N6	115.2 (9)
C5—N3—H3	118.3	N4—C16—C15	122.1 (10)
C6—N3—H3	118.3	N6—C16—C15	122.6 (10)
C16—N4—C12	118.0 (9)	N6—C17—C18	114.8 (9)
C16—N4—Ag2 <sup>iv</sup>	127.9 (7)	N6—C17—H17A	108.6
C12—N4—Ag2 <sup>iv</sup>		C18—C17—H17A	108.6
_	114.0 (7)		
C21—N5—C22	119.9 (9)	N6—C17—H17B	108.6
C21—N5—Ag2	117.9 (7)	C18—C17—H17B	108.6
C22—N5—Ag2	121.3 (7)	H17A—C17—H17B	107.5
C16—N6—C17	122.3 (10)	C19—C18—C22	119.0 (10)
C16—N6—H6	118.9	C19—C18—C17	119.8 (9)
C17—N6—H6	118.9	C22—C18—C17	121.2 (9)
N1—C1—C2	129.9 (13)	C18—C19—C20	119.5 (10)
N1—C1—H1	115.1	C18—C19—H19	120.2
C2—C1—H1	115.1	C20—C19—H19	120.2
C1—C2—C3	114.1 (12)	C19—C20—C21	119.1 (10)
C1—C2—H2	123.0	C19—C20—H20	120.4
C3—C2—H2	123.0	C21—C20—H20	120.4
C2—C3—C4	120.6 (12)	N5—C21—C20	121.0 (10)
C2—C3—H3A	119.7	N5—C21—H21	119.5
C4—C3—H3A	119.7	C20—C21—H21	119.5
C3—C4—C5	119.0 (11)	N5—C22—C18	121.4 (10)
C3—C4—H4	120.5	N5—C22—H22	119.3
C5—C4—H4	120.5	C18—C22—H22	119.3
N3—C5—N1	117.8 (9)	03—S1—01	
	* /		114.7 (5)
N3—C5—C4	122.8 (10)	03—S1—02	115.2 (5)
N1—C5—C4	119.4 (11)	01—S1—02	114.6 (5)
N3—C6—C7	114.7 (10)	O3—S1—C23	103.0 (5)
N3—C6—H6A	108.6	O1—S1—C23	103.6 (5)
C7—C6—H6A	108.6	O2—S1—C23	103.6 (5)
N3—C6—H6B	108.6	F2—C23—F3	108.3 (9)
C7—C6—H6B	108.6	F2—C23—F1	107.7 (9)
H6A—C6—H6B	107.6	F3—C23—F1	107.5 (9)
C8—C7—C11	116.8 (10)	F2—C23—S1	110.9 (8)
C8—C7—C6	119.6 (10)	F3—C23—S1	110.9 (8)
C11—C7—C6	123.5 (10)	F1—C23—S1	111.3 (8)
C9—C8—C7	121.8 (11)	O6—S2—O5	118.1 (6)
C9—C8—H8	119.1	O6—S2—O4	114.7 (5)
C7—C8—H8	119.1	O5—S2—O4	112.9 (6)
C8—C9—C10	117.9 (10)	O6—S2—C24	104.9 (6)
C8—C9—H9	121.1	O5—S2—C24	102.1 (6)
C10—C9—H9	121.1	O4—S2—C24	101.5 (6)
N2—C10—C9	123.0 (10)	F5—C24—F4	108.3 (11)
N2—C10—C)	118.5	F5—C24—F6	110.3 (11)
112	110.3	13-02-10	110.5 (11)

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C9—C10—H10	118.5	F4—C24—F6	107.1 (11)
N2—C11—C7	122.7 (10)	F5—C24—S2	112.9 (9)
N2—C11—H11	118.7	F4—C24—S2	110.2 (9)
C7—C11—H11	118.7	F6—C24—S2	107.8 (9)
$N2^{i}$ — $Ag1$ — $Ag2$ — $N4^{ii}$	0.5 (3)	C12—C13—C14—C15	-1.5 (19)
N1—Ag1—Ag2—N4 <sup>ii</sup>	177.3 (3)	C13—C14—C15—C16	0.4 (17)
$N2^{i}$ — $Ag1$ — $Ag2$ — $N5$	-166.0(3)	C12—N4—C16—N6	-179.8(9)
N1—Ag1—Ag2—N5	10.9 (3)	Ag2 <sup>iv</sup> —N4—C16—N6	-2.3(14)
N2 <sup>i</sup> —Ag1—N1—C1	110 (3)	C12—N4—C16—C15	-1.6(15)
Ag2—Ag1—N1—C1	82.1 (9)	Ag2 <sup>iv</sup> —N4—C16—C15	175.8 (8)
N2 <sup>i</sup> —Ag1—N1—C5	-67 (3)	C17—N6—C16—N4	-164.2 (9)
Ag2—Ag1—N1—C5	-94.4 (7)	C17—N6—C16—C15	17.7 (16)
N4 <sup>ii</sup> —Ag2—N5—C21	-51.1 (13)	C14—C15—C16—N4	1.2 (16)
Ag1—Ag2—N5—C21	93.7 (8)	C14—C15—C16—N6	179.2 (10)
N4 <sup>ii</sup> —Ag2—N5—C22	118.2 (10)	C16—N6—C17—C18	-89.4 (13)
Ag1—Ag2—N5—C22	-96.9 (8)	N6—C17—C18—C19	176.1 (10)
C5—N1—C1—C2	1 (2)	N6—C17—C18—C22	-5.8 (16)
Ag1—N1—C1—C2	-175.3 (12)	C22—C18—C19—C20	-2.8(15)
N1—C1—C2—C3	-1 (2)	C17—C18—C19—C20	175.3 (10)
C1—C2—C3—C4	0.9 (19)	C18—C19—C20—C21	-0.2 (16)
C2—C3—C4—C5	-0.3 (19)	C22—N5—C21—C20	-2.4(16)
C6—N3—C5—N1	164.4 (10)	Ag2—N5—C21—C20	167.1 (8)
C6—N3—C5—C4	-16.9(17)	C19—C20—C21—N5	2.8 (17)
C1—N1—C5—N3	178.2 (11)	C21—N5—C22—C18	-0.7(15)
Ag1—N1—C5—N3	-5.1 (13)	Ag2—N5—C22—C18	-169.8(8)
C1—N1—C5—C4	-0.5 (15)	C19—C18—C22—N5	3.3 (15)
Ag1—N1—C5—C4	176.2 (8)	C17—C18—C22—N5	-174.8(10)
C3—C4—C5—N3	-178.6 (11)	O3—S1—C23—F2	61.0 (9)
C3—C4—C5—N1	0.0 (17)	O1—S1—C23—F2	-58.8(9)
C5—N3—C6—C7	95.1 (14)	O2—S1—C23—F2	-178.7(8)
N3—C6—C7—C8	170.4 (10)	O3—S1—C23—F3	-178.7(8)
N3—C6—C7—C11	-6.0(17)	O1—S1—C23—F3	61.6 (9)
C11—C7—C8—C9	-1.6 (16)	O2—S1—C23—F3	-58.3 (9)
C6—C7—C8—C9	-178.3 (11)	O3—S1—C23—F1	-59.0 (9)
C7—C8—C9—C10	1.4 (17)	O1—S1—C23—F1	-178.7(8)
C11—N2—C10—C9	2.0 (16)	O2—S1—C23—F1	61.3 (9)
Ag1 <sup>iii</sup> —N2—C10—C9	175.4 (8)	O6—S2—C24—F5	-177.0(10)
C8—C9—C10—N2	-1.6 (17)	O5—S2—C24—F5	59.3 (11)
C10—N2—C11—C7	-2.3(15)	O4—S2—C24—F5	-57.4 (11)
Ag1 <sup>iii</sup> —N2—C11—C7	-175.5 (8)	O6—S2—C24—F4	-55.7 (11)
C8—C7—C11—N2	2.1 (16)	O5—S2—C24—F4	-179.3 (9)
C6—C7—C11—N2	178.7 (11)	O4—S2—C24—F4	64.0 (10)
C16—N4—C12—C13	0.5 (15)	O6—S2—C24—F6	60.9 (10)
Ag2 <sup>iv</sup> —N4—C12—C13	-177.3 (9)	O5—S2—C24—F6	-62.8 (10)
N4—C12—C13—C14	1.1 (17)	O4—S2—C24—F6	-179.5 (8)
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Symmetry codes: (i) -x+1, y+1/2, -z+1/2; (ii) -x, y+1/2, -z+1/2; (iii) -x+1, y-1/2, -z+1/2; (iv) -x, y-1/2, -z+1/2.

#### Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	$H\cdots A$	D··· $A$	<i>D</i> —H··· <i>A</i>
N3—H3···O4	0.88	2.20	3.021 (12)	156
N6—H6···O2 <sup>iv</sup>	0.88	2.42	3.159 (12)	142
C1—H1···O1	0.95	2.56	3.389 (16)	146
C6—H6 <i>A</i> ···F6 <sup>v</sup>	0.99	2.55	3.282 (15)	131
C9—H9···O3 <sup>vi</sup>	0.95	2.44	3.329 (14)	156
C10—H10···O1 <sup>iii</sup>	0.95	2.57	3.373 (14)	142
C12—H12···O4 <sup>vii</sup>	0.95	2.51	3.331 (15)	145
C17—H17 <i>A</i> ···O3 <sup>iv</sup>	0.99	2.42	3.186 (14)	134
C21—H21···F6 <sup>i</sup>	0.95	2.54	3.325 (14)	140

Symmetry codes: (i) -x+1, y+1/2, -z+1/2; (iii) -x+1, y-1/2, -z+1/2; (iv) -x, y-1/2, -z+1/2; (v) x, -y+3/2, z+1/2; (vi) x+1, -y+3/2, z+1/2; (vii) x-1, y, z.